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Localized Voronoi analysis of quenched liquid configurations TRAVIS PEERY, NICOLAS BOCK, GIULIA DE LORENZI-VENNERI, DUANE WALLACE, Theoretical Division, Los Alamos National Laboratory, ERIK HOLMSTROM, Instituto de fisica, Universidad Austral de Chile — We developed a set of *localized* statistical tools to explore and characterize condensed matter particle configurations, particularly amorphous distributions associated with the liquid state. Typically global measures of atomic packing are used to characterize atomic configurations, such as pair distribution functions. For large systems, such calculations can be computationally expensive and tend not to be sensitive to localized symmetries. Our localized tools are based upon the geometric or topological analysis of (static) atomic arrangements using Voronoi polyhedra. As each atom in the configuration has a unique Voronoi polyhedron defined by its near neighbors, our tools can describe the geometry and symmetry of local neighborhoods. We have defined, for example, a local, Shannon-type entropy for the Voronoi coordination number for each atom in a 500-atom, monatomic system. This *localized* entropy tool was able to find small (9–40 atom) crystallites or regions of high symmetry in an otherwise random 500-atom configuration quenched from a liquid MD state. These tools will help to define and characterize not only random liquid state configurations and the minimum structures associated with liquid potential energy surfaces, but also the symmetry properties of the quenching process itself.

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